REPORT of March 7th MEETING of the FFCC on Predictive Codes

A videoconference of the Fusion Facilities Coordinating Committee was held on March 7th. This meeting was in response to a request from John Willis. On February 14th, John sent an email to the chair of the FFCC requesting "a televideo discussion of transport code use and plans for the three major facilities. I suggest that such a discussion probably should seek participation from both users & code developers on DIII-D, C-Mod, and NSTX. In addition to their roles on the major facilities, it would be good code developers to address the use of these codes on alternate experiments. Finally, since these proposed transport efforts should carry forward to the NTCC it would be good to hear from that perspective as well. In the end, I would like to have an assessment from the FFCC on what activities and developments people are in agreement on, what are differences of opinion, and what are recommended actions."

In response to this request, an agenda for the meeting was set up (see Appendix A.). Broader participation in this meeting was necessary and achieved in the televideo. In addition to the FFCC members from GA, MIT, PPPL, ORNL and Columbia, we had participation from Lehigh University, ORNL, LLNL, Univ. of Maryland, Univ. of Colorada, Univ. of Texas, and Georgia Tech. The first part of the meeting was a discussion of "Users Needs". Prior to the meeting, M. Murakami (DIII-D), M. Greenwald (C-Mod), S. Kaye (NSTX), B.Dorland (Univ.) and J. Cary (Univ.-2) described the needs of their facilities or communities and distributed their reports to all of the participants. R. Hawryluk worked with this group to develop a composite document of the needs for all of these groups. That summary document is attached. Due to the limited time available, that summary should be viewed as a snapshot in time reflecting the opinions of the people sampled. Not enough time was available to iterate with the participants and develop a comprehensive requirements document. Over a hundred "needs" were identified. A substantial number of the needs were common to all of the groups; however, not all reflecting, in part, different programmatic priorities as well as different technical needs and emphasis on short versus longer-term issues. Nonetheless in the panel discussion, members representing the users' needs indicated that there was significant agreement on the needs and fair consensus. Though many issues came up in the discussion regarding longer-term needs, the focus of the group was on near-term needs in support of the facilities. The research program on DIII-D is the largest driver for near term predictive modeling support in support of scenario development for the AT program during the next six to twelve months and an internal assessment in 2002 of what additional hardware capabilities are needed. All of the facilities are focussed on the FESAC assessment in 2004,which is a longer-term need compared with what DIII-D described.

In the second part of the agenda, a series of presentations by "code developers" were given. This was an excellent review of the status of the various codes and provided insight into areas requiring additional effort. Most of the presenters have provided copies of their talks to the participants.

After the presentations, the FFCC discussed the issues and developed a framework for considering both the near-term and long-term issues. The Projects, composed of national teams, need certain tools by certain dates to support their research programs. They need the flexibility to address their high priority concerns within their resources. Indeed this has traditionally been the way analysis codes, predictive codes and physics modules have been developed. However, it is also clear that there are long-term developments of importance not only to the Projects but also to the Theory community which need to be supported by DOE and which go beyond the traditional focus of the Projects. The issue is how to ensure that the near-term efforts by the Projects support our long term needs and also how to get near term benefits from some of the development work being funded with a longer term perspective. At the same time, we do not want to create a paralyzing bureaucracy as to stifle initiative and innovation and delay the implementation of much needed upgrades.

A vital need, on which there is broad consensus of both general approach and specific implementation, is for there to be clearly defined input and output data structures for the codes and a standard, well-specified calling interface for reading and writing data. MDSplus has been adopted throughout the US as the underlying database interface. Jointly agreed data structures (MDSplus "trees") have been specified already for a significant number of the commonly-used codes: (TRANSP, EFIT, PEST, ...) allowing them to be used at all facilities, once that device-specific data is removed from the codes and placed into the data-structure. This approach makes it possible for a user at a lab or university to run the code with a minimum of setup and code modification, and to develop new modules that access the data transparently.

The facilities have also identified activities in the area of software sharing with would benefit all of the Projects and facilitate both the input of data and output of results for further processing. Such activities should be encouraged.

Since the facilities have pressing project-specific near-term needs they need to devote appropriate resources to this directed development. Wherever possible, new modules that incorporate the latest physics should be written in accordance with the NTCC standards such that after the code is benchmarked and validated it is available to all of the code frameworks or users within the community.

It is not recommended that we immediately down-select to one code framework. A great deal of effort has been expended on the existing code frameworks, which are an integral part of the experimental programs. Switching between codes will undoubtedly involve some short-term dislocation, which is not acceptable in some areas. Nevertheless, there is consensus on the following values:

1. A broad user base beyond the home institution is helpful both to assure validation of the code and to share the expenses of code development and maintenance.
2. Some level of assistance and support to users is probably necessary to attract and sustain such a user base.
3. Transport Code(s), which are capable of prediction as well as analysis, were emphasized.
4. Groups should work together on common objectives wherever possible.

Three specific categories of approach to the longer-term development were identified: (1) Continued development of existing codes. (2) The NTCC framework. (3) The GA/LLNL Corsica/ONETWO proposal. Not all of the good ideas presented can be done within the resources available. Leaders of the facilities requested a role in setting the priorities for these activities to help ensure that the long term goals are practical and supportive of the programs' long term vision. Just as it is important that software development being done by the Facilities should have the long term needs of the community in mind, similarly the software development being done by the community should have the needs of the Facilities and of the wider program in mind.

It is clear that continued development of existing codes (1) is beneficial and inevitable especially for codes that serve a large, multi-institutional user base. It should be done in such a way as to evolve the codes as far as possible towards supporting and taking advantage of the common input/output data structures, and of the module specifications of NTCC.

At present NTCC (2) is promising but is funded in such a sparse manner as to preclude intensive development efforts. There is a need for NTCC to identify one or two nearer-term objectives so as to bring the benefits of its general principles to "market" in the form of a usable "product". This could convince the community at large of the value of those benefits, and thereby recruit active supporters and, perhaps more importantly, computationalists, to expand its activities. Proposals to develop approximately along this path were discussed at the meeting. We believe that significant evolution of the NTCC structure will be necessary if it is to adopt this approach. It will need to become more focussed, with leadership, accountability, a specified objective and schedule, and with participants funded at a higher fractional level so that they have a significant commitment to, and time for, the project. At this meeting, it was indicated that a PAC would be formed for the NTCC. This could be a vehicle for obtaining input from the large facilities, and for implementing an accountable management structure.

Several (but not all) members of the FFCC (Ben Carreras, Richard Hawryluk, Richard Hazeltine, Ian Hutchinson, Gerald Navratil, and Martin Peng) felt that the Corsica/ONETWO proposal (3) would not address the near-term high-priority modeling needs identified by the DIII-D team, which emphasized results within this year. Nor does it currently appear likely to attract users from other facilities, because of the investment of other institutions in other interpretive and predictive codes. While the Committee certainly supports the individual projects pursuing work that is necessary to meet the project-specific goals, we believe that the greatest leverage is to be gained by using the extra, but limited, resources to fund further development of widely-based tools for even wider community use. Further discussion and follow up on comments/issues associated with all three options is required to define a long term strategy.

Appendix A.
Agenda:

Panel discussion of Users Needs: 12:00-1:00 pm

Panel:

DIII-D	M. Murakami	
C-Mod	M. Greenwald	
NSTX	S. Kaye	
University Users:	B. Dorland	
Data Interface:	M. Greenwald	
	J. Cary	

Presentation of code options to address users' needs:

Corsica	L. Lodestro	1:00-1:20
ONETWO	H. St John	1:20-1:40
Baldur	G. Bateman	1:40-2:00
NTCC	R. Cohen	2:00-2:20
Transp	D. McCune	2:20-2:40
TSC	S. Jardin	2:40-3:00
Whist	W. Houlberg	3:00-3:20
TBD (solver)	W. Horton	3:20-3:40
Break		3:40-3:55
FFCC Discussion		3:55-6:00
Adjourn		6:00

General Remarks:

Program would benefit from enhancements and additions to existing codes as well as others. (C-Mod, DIII-D, NSTX, Univ., Univ-2)

Need to reduce the effort required to apply codes to the experiments.
(C-Mod ,DIII-D, NSTX, Univ., Univ.-2)

Each experiment should have access to and can be analyzed with all the relevant codes and where each code can be run against data from all the experiments. (C-Mod, NSTX) (DIII-D, Univ. views as a longer term requirement) (Univ-2. Some prioritization will be necessary.)

The advantages of sharing software between major facilities are clear.
(C-Mod, DIII-D, Univ., Univ.-2, NSTX)

Serve the needs for both experimental users and modelers; analysis and simulation in the same or well coupled codes. (DIII-D, C-Mod, NSTX, Univ.,Univ-2)

Efficient interface from data through to transport code results (DIII-D, C-Mod, NSTX Univ.)

Existing codes must be maintained while enhancements are incorporated and changes must be backward compatible. (DIII-D, C-Mod agrees up to a point, sometimes a clean break must be made, NSTX agrees with compatibility ensured through data interfaces)
- developmental stability is a medium to long-term goal (Univ.)

Stability, versioning, snapshots available through CVS (Univ-2, C-Mod, Univ.,NSTX)

Transition from time-dependent analysis to simulation mode. (DIII-D, NSTX, C-Mod, Univ.-2)

Avoid discipline specific software. Stick with industry standards. (Univ-2,Univ.)

Community owned codes that can be community modified (Univ-2,Univ.)

New approaches in parallel with supporting one or two mainlines (Univ-2, Univ.)

1. Physics modules

Users should be able to choose from a wide range of physics modules. (NSTX, C-Mod, Univ., Univ.-2)
- Well defined and documented mechanism for module addition (Univ-2, C-Mod, Univ., NSTX)
- Effort on modules library as well as a national transport code should support new approaches to old problems. (Univ., Univ.-2, NSTX)

RF source modules:
ICRF full-wave (as in for example TORIC, PICES) (C-Mod, DIII-D, NSTX)
Fokker-Planck (FPPRF) (C-Mod, NSTX)
Lower Hybrid (LSC, ACCOME) (C-Mod)
CURRAY (DIII-D, NSTX)
HPRT (NSTX)
ECH & CD modeling. (DIII-D)

Up-to-date neutral transport solver. (C-Mod, DIII-D, NSTX)
- Better treatment of neutral dynamics in edge including flow damping and improved resolution .(C-Mod)
- Halo neutrals (DIII-D) (exists in TRANSP,NSTX)

Treatment/integration of SOL/divertor plasma. (C-Mod, DIII-D) [Longer term]

Atomic physics for high Z impurities (Molybdenum). (C-Mod)

Micro-stability calculations based on experimental profiles and magnetic geometry. (C-Mod) [Longer term]
- This is available now for GS2. (Univ.)

(If feasible) Non-linear turbulence calculations based on experimental profiles and magnetic geometry. (We imagine that this would be used to generate synthetic fluctuation data to compare to experiments.) (C-Mod) [Longer term]
- This is coming on line, thus it is short term. (Univ.)

Most advanced source modules are required particularly in analysis code but there is a tradeoff between speed versus accuracy. (DIII-D, Univ.)

Need state of art transport models to test most advanced ideas (DIII-D, Univ., NSTX) [This activity is both short and longer terms because of continuously evolving nature]

Time-dependent current profile analysis mode is required (DIII-D, NSTX)
- Internal loop voltage analysis mode. (DIII-D)

State of the art neoclassical transport model. (DIII-D, C-Mod, Univ.)
- NCLASS including low aspect ratio (NSTX, Univ.)
- Orbit loss at edge for bootstrap current model (DIII-D, Univ.)

MHD-enhanced transport modeling. (DIII-D)
- sawteeth model included but not others (DIII-D, NSTX, C-Mod)

NBH &CD using detailed beam physics. (DIII-D,NSTX)
- incorporate low aspect ratio relevant FLR effects in Monte-Carlo calculations, and comprehensive atomic physics package (NSTX)
- Specify structures that can cause orbit loss. (NSTX)

NBH &CD using Fokker-Plank or orbit-averaging models for fast ("between-shots") analysis. (DIII-D, NSTX)

Fusion neutrons (e.g., including beam-beam neutrons) (DIII-D, NSTX)

Magnetic diffusion calculations including eddy currents in passive plates. (NSTX)

Robust and fast equilibrium solver. (NSTX, DIII-D, C-Mod)
- This should include solvers like TOQ, JSOLVER or QSOLVER rather than only EFIT. (Univ.)

2. Computational and grid/resolution

There is substantial interest in transport codes, which allow much higher or variable resolution in the plasma edge. (C-Mod, DIII-D, Univ.)

Rapid build process, minimized dependencies (Univ-2, C-Mod)
- Robust rebuild, rapid long-term goal. (Univ.)

Regridding on the fly (Univ-2)

Inherently modular, so that modules can be easily stripped out and reused elsewhere (Univ-2, C-Mod, Univ.)

Weakly coupled systems allowing changeout or modification (Univ-2, C-Mod)

3. Predictive/analysis mode

It would be desirable for the transport codes to run in both predictive and analysis modes on a channel by channel basis (ie particle, electron energy, ion energy, impurity). (C-Mod, DIII-D, NSTX, Univ. Univ.-2)

- adjust boundary location to address model limitations in edge region (NSTX, Univ.)
    - Must do better eventually (Univ.-2)
- phase in predictive capability commensurate with physics model capability (i.e., heat, momentum, particle, impurity) (NSTX)

They should use existing data input and pre-processing capabilities and allow users to select at run time, the physics modules which would run in analysis mode and those which would run in predictive mode (C-Mod, DIII-D, Univ.-2, NSTX)

- Agree with run-time selection of modules but disagree with constraint to existing data input and pre-processing capabilities. (Univ.)

Support both single time-slice as well as time dependent. (DIII-D, NSTX)

Free boundary operation. (DIII-D, C-Mod, Univ as an option)

Fixed boundary adequate for transport-specific calculation. (NSTX)

Benchmark with other codes and experiment. (DIII-D, C-Mod, NSTX, Univ.)

Talk to experiments via one transport code (Univ.)

- DIII-D does not necessarily agree; the choice should be left for users (DIII-D)
- More than one community code - accommodate diverse styles, competition (Univ-2)

4. Ease of use issues -

Decrease the effort in installing, adapting and maintaining codes, which can tax the resources of any group and represent a barrier to their wide use. (C-Mod, Univ.-2)

- emphasis should be placed on making it as easy as possible. (Univ.)

The users need to understand the physics content of the codes they use and need to work collaboratively with the developers. (C-Mod, DIII-D, NSTX)

- A goal should be that the code will also be useful to a wide group of users who were not involved in the development. (Univ-2)

It is a requirement that codes read and write to MDSplus servers. (C-Mod, DIII-D, NSTX)

- Universities want whatever exists to read the experimental data. If that is MDSplus, then we agree. (Univ.)
- True. We should define (independently of implementation) an interface for interacting with the data typical of our field. (Univ.-2)

Access to experimental data should be more uniform. (Univ, C-Mod.)

Bulk transfers of data to local machine (Univ-2, C-Mod skeptical of this approach, NSTX disagrees)

Ability to store data locally in self describing files (Univ.-2)

Ability to read from and write to multiple data storage mechanisms from single interface (Univ.-2)

Data should be provided with generic services - interpolation, name translation (Univ.-2, Univ.)

Secure access to data (Univ.-2, C-Mod)
- add automatic fail switch along with name service for finding available servers. (Univ.-2)

It is crucial to remove all machine specific or run specific data from the codes and move them into the MDSplus data trees. (C-Mod, DIII-D, NSTX)

Comprehensive GUIs for data preparation. (NSTX, C-Mod)
- Web based GUI's for ease of access (Univ-2)

Control of run options through an input file or GUI and run as a batch job. (NSTX, C-Mod, Univ.-2)
- allow codes to be steered. (Univ.-2)

Use Review Plus as the primary display tool. (DIII-D) [This meant to be DIII-D specific, and data in the MDSplus]
- Use of multiple tools for display, with emphasis on those based on freeware (Univ-2)

Flexible post-processors for viewing, manipulating results, comparing to measurements. (NSTX, DIII-D, C-Mod, Univ.,Univ.-2)

By sharing MDSplus tree structures, a mechanism for linking results of codes is created automatically which is needed. (C-Mod, DIII-D, NSTX)
- Must have common names for data access and re MDSplus, standardize on tree structure. (Univ.-2)

Use of relational databases to track code runs. (C-Mod, DIII-D, Univ., NSTX)
- track code-run characteristics (Univ.-2)

Where possible, it would seem desirable to minimize the number of installations that must be maintained. (C-Mod, NSTX, Univ.)
- Instead run code on whatever platform they have chosen. (Univ.-2)

Tested by a large number of users (NSTX, DIII-D, C-Mod)
- Long term goal which should not preclude rapid deployment of new modules. (Univ.)

Portability (DIII-D, C-Mod, NSTX, Univ.)

Maintainability including timely response (either on-site or off-site support) (DIII-D, C-Mod, Univ., Univ.-2)

User-friendliness. (DIII-D, C-Mod, NSTX. Univ.-2)
- ease of use (Univ., Univ.-2, NSTX)
- adequate documentation (Univ., Univ.-2, NSTX)
- avoidance of excessive old or new software (Univ., Univ.-2, NSTX)
- web based documentation detailing precise calls rather than just available functions (Univ.-2, C-Mod, NSTX)

Diagnostic simulations (NSTX, DIII-D, C-Mod)

Adequate access to experimental data (Univ., C-Mod, NSTX, Univ.-2)

Full access to source code, to allow exploratory modifications. (Univ., NSTX)
- Code must be supported by code development system that can be accessed by users and developers. (NSTX, C-Mod, Univ.-2)

Adequate support to develop successful new idea into production modules. (Univ., Univ.-2)

5. Longer Term Features

Restart capability. (DIII-D, NSTX, Univ.-2) [near-term for some of the codes]

Physics-based transport with dynamically evolving ExB shear. (DIII-D, C-Mod, NSTX Univ.-2)

Coupled MHD stability. (DIII-D, NSTX, Univ.-2)

Core/edge coupling. (DIII-D, C-Mod, Univ.-2)
- not at this stage (NSTX)

Use of parallelization to speed up code modules. (DIII-D, NSTX, Univ.-2)

Free-boundary equilibrium with circuit equations. (DIII-D, C-Mod, Univ.-2)
- used for scenario development and device upgrade (NSTX, Univ.-2)

NBI full orbit tracking. (NSTX, Univ.-2)

6. Time scale for code enhancments

Progress check points for AT program (2001) (DIII-D)

Analysis in support for proposals (2002) (DIII-D)

FESAC assessment (2004) (DIII-D, NSTX)

In support of NSTX experiments, need enhanced modules appropriate for low aspect ratio interpretive code. (2001) (NSTX)
- Use of enhanced modules for partial predictive capability (2001) (NSTX)